

AD

2

TECHNICAL REPORT 88-10

OCTANOL WATER PARTITION COEFFICIENTS OF  
SURFACE AND GROUND WATER CONTAMINANTS FOUND AT MILITARY INSTALLATIONS

MICHAEL A. MAJOR, Ph.D.

NOVEMBER 1989

AD-A228 860

DTIC  
ELECTE  
NOV 1 1990  
S B D  
Co

U S ARMY BIOMEDICAL RESEARCH & DEVELOPMENT LABORATORY  
Fort Detrick  
Frederick, MD 21701-5010

Approved for public release;  
distribution unlimited.

U S ARMY MEDICAL RESEARCH & DEVELOPMENT COMMAND  
Fort Detrick  
Frederick, MD 21701-5012



## NOTICE

### Disclaimer

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorized documents.

### Disposition

Destroy this report when it is no longer needed. Do not return it to the originator.

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
1a. REPORT SECURITY CLASSIFICATION Unclassified			1b. RESTRICTIVE MARKINGS		
2a. SECURITY CLASSIFICATION AUTHORITY			3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited		
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE					
4. PERFORMING ORGANIZATION REPORT NUMBER(S)			5. MONITORING ORGANIZATION REPORT NUMBER(S)		
6a. NAME OF PERFORMING ORGANIZATION U.S. Army Biomedical Research and Development Laboratory		6b. OFFICE SYMBOL (If applicable) SGRD-UBG-E	7a. NAME OF MONITORING ORGANIZATION		
6c. ADDRESS (City, State, and ZIP Code) Fort Detrick Frederick, MD 21701-5010			7b. ADDRESS (City, State, and ZIP Code)		
8a. NAME OF FUNDING/SPONSORING ORGANIZATION U.S. Army Medical Research and Development Command		8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER		
8c. ADDRESS (City, State, and ZIP Code) Fort Detrick Frederick, MD 21701-1010			10. SOURCE OF FUNDING NUMBERS		
		PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO.
11. TITLE (Include Security Classification) Octanol/Water Partition Coefficients of Installation Surface and Ground Water Contaminants					
12. PERSONAL AUTHOR(S) Michael A. Major, Ph.D.					
13a. TYPE OF REPORT Technical		13b. TIME COVERED FROM Jun 88 to Oct 89	14. DATE OF REPORT (Year, Month, Day) 1989 November		15. PAGE COUNT
16. SUPPLEMENTARY NOTATION					
17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)		
FIELD	GROUP	SUB-GROUP	Octanol/water partition coefficients		
			Kow		
			Log P.		
19. ABSTRACT (Continue on reverse if necessary and identify by block number)					
<p>An octanol/water partition coefficient (<math>K_{ow}</math>) is the ratio of the concentrations of a solute in the two phases that are created when water containing the solute is extracted with octanol. <math>K_{ow}</math> values are of considerable use in an estimating other equilibrium constants needed for predicting the fate of chemicals in the environment. This paper reports <math>K_{ow}</math> values for a number of compounds, some of which are unique to the military. The values have been selected from government reports and the open literature or determined in the U.S. Army Biomedical Research and Development Laboratory.</p>					
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT <input checked="" type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT. <input type="checkbox"/> DTIC USERS			21. ABSTRACT SECURITY CLASSIFICATION Unclassified		
22a. NAME OF RESPONSIBLE INDIVIDUAL Michael A. Major, Ph.D.			22b. TELEPHONE (Include Area Code) 301/663-2538		22c. OFFICE SYMBOL SGRD-UBG-E

DD Form 1473, JUN 86

Previous editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE

# TABLE OF CONTENTS

	<u>Page</u>
EXECUTIVE SUMMARY.....	1
INTRODUCTION.....	1
DERIVATIVES OF METHYLPHOSPHONIC ACID.....	2
METHYLMERCURIES AND DIMETHYLMERCURY.....	4
COMPOUNDS OF ARSENIC.....	5
ELEMENTAL METALS.....	5
OTHER COMPOUNDS FOR WHICH $K_{OW}$ IS NOT APPLICABLE.....	6
TABLE OF $LOGK_{OW}$ VALUES.....	6
REFERENCES.....	13
APPENDIX A.....	16
DISTRIBUTION LIST.....	17

Accession For	
NTIS GRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A-1	

## EXECUTIVE SUMMARY

This report summarizes the octanol/water partition coefficients ( $K_{ow}$ ) for a variety of substances frequently encountered as environmental pollutants that are unique to or of particular interest to the military. Sources of the data are experimental values published in the open literature or in government reports, and values determined experimentally in this Laboratory. The purpose of the report is to contribute to the establishment of a  $K_{ow}$  data base to be used in predictive models of transport and transformation in the environment; it will aid in the assessment of possible ecological and health impacts due to past or present military activities.

## INTRODUCTION

The ecological and health effects of chemical pollutants disseminated in association with the production and use of munitions and chemical agents are an important concern of the U.S. Army Medical Research and Development Command. The problem is complex from a chemical standpoint because of the large variety of toxic chemicals associated with their manufacture. The situation is further complicated by the physical and chemical transformations these compounds undergo in storage, during use and in the environment. Moreover, much of the current contamination was generated by a succession of government and corporate laboratories; proper containment procedures were yet to be developed and records were sometimes inadequate.

Octanol/water partition coefficients ( $K_{ows}$ ) are of considerable use for deriving other equilibrium constants needed to predict the fate of chemicals in the environment<sup>1</sup>. Values of  $K_{ow}$  can be estimated by a variety of calculations<sup>2</sup> but are more accurately derived experimentally. The earliest experimental method relied on establishing an equilibrium of solute between the immiscible distribution solvents octanol and water. In this "shake flask" method, octanol and water containing the solute are vigorously shaken until equilibrium is achieved and the two phases allowed to separate; the concentration of the solute in the octanol divided by that in water is the  $K_{ow}$ . This method, although still the standard, is time-consuming and presents problems whenever very large or very small  $K_{ows}$  are encountered. A more convenient method<sup>3</sup> has been developed that relies on the relationship between a compound's octanol/water partition coefficient and its retention time in reverse phase high-performance liquid chromatography (HPLC). In this method the known  $\log K_{ow}$  values for a series of standards are plotted against the logarithms of their corrected HPLC retention times, and the slopes of such relationships are determined by linear regression.  $K_{ow}$  values for compounds similar to the standards can then be accurately estimated from their retention times by interpolation. While this solves many of the problems associated with the shake flask method, it is only accurate when the compounds used as standards and the unknowns contain similar functional groups and have similar

polarity. Compounds with very high  $K_{ow}$  values require a special modification of the shake flask method. In this technique the combined octanol/water phases are carefully layered to avoid emulsion, the solute added and the mixture slowly stirred for several days to achieve equilibrium. The phases are then analyzed and the  $K_{ow}$  determined as in the shake flask procedure.

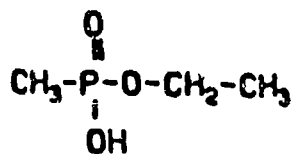
Regressions have been established between  $K_{ow}$  and solubility, adsorption on soil and uptake by aqueous organisms<sup>1</sup>. Due to the utility of  $K_{ow}$  as a predictive tool, values for many compounds have been determined, and a convenient listing of these was provided a decade ago by Hansch and Leo<sup>2</sup>. In addition, relatively accurate estimates of  $K_{ow}$  can often be obtained by calculations that utilize fragment analyses and by regression equations that relate  $K_{ow}$  to the partition coefficient of solutes between water and other solvents<sup>2</sup>.

The listing we provide here is in response to a U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) request for  $K_{ow}$  values for the compounds found in Appendix A. The reported values are experimentally derived but estimation methods have been used to pick best values among widely differing published  $K_{ows}$ . Laboratory determinations of  $K_{ow}$  were performed in-house by the HPLC retention time method of Harnisch<sup>3</sup> when literature results were not available.  $K_{ow}$  determinations for compounds with known values were also performed for standardization, and as a check on the accuracy of the laboratory procedures.

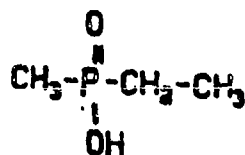
To assist the reader in identifying the compounds of interest, chemical structures are provided and related compounds are handled as subgroups. Compounds not found in water in the form listed, such as lewisite, and compounds that are ions under normal conditions (pH values between 5 and 9) do not have meaningful  $K_{ow}$  values. These compounds are identified in the text.

#### DERIVATIVES OF METHYLPHOSPHONIC ACID

Owing to changes in the rules of nomenclature one may experience some ambiguity as to the structure of these compounds. Under older rules of nomenclature<sup>4</sup>, ethyl methylphosphonate and ethyl methylphosphonic acid would denote the monoethyl ester and the "secondary phosphonic" (really a phosphinic) acid shown here.

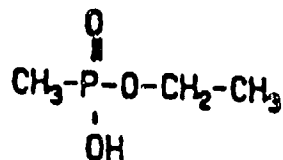


Ethyl half ester



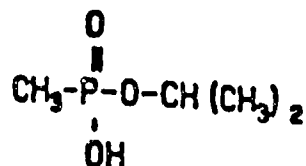
Secondary phosphonic acid

Under current rules<sup>5</sup> the latter compounds are named phosphinic acids, and the terms ethyl methylphosphonate and ethyl methylphosphonic acid now designate the same compound.



Ethyl methylphosphonate/Ethyl methylphosphonic acid

Similar nomenclature applies to isopropyl methylphosphonate (isopropyl methylphosphonic acid).

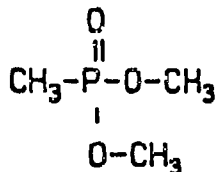


Isopropyl methylphosphonate/Isopropyl methylphosphonic acid

Apparently USATHAMA (Appendix A) used the suffix "ate" to indicate the salt form and the "acid" ending to indicate an undisassociated Lowry-Bronsted acid. The question of whether these compounds exist in the ionized or un-ionized form is important, for if they are ionized they will remain almost exclusively in the aqueous phase and will not have a demonstrable  $K_{ow}$ . Acid strength of organic acids decreases with increasing length of the attached hydrocarbon chains. Therefore, since the  $pK_a$  of the largest phosphonic acid on our list (isopropyl methylphosphonic acid) is lower than 5, it follows that it and the other phosphonic acids would be almost completely ionized under normal environmental conditions.

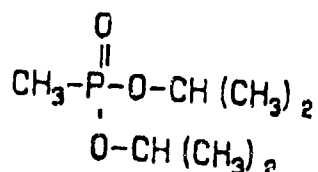
Experiments in our laboratory<sup>6</sup> using the titration method of Rosenblatt and Davis<sup>7</sup> have demonstrated a  $pK_a$  for isopropyl methylphosphonate of 2.41. Kosolapoff<sup>4</sup> reports a  $pK_a$  for methylphosphonic acid of 2.35. We therefore consider both ethyl methylphosphonate and isopropyl methylphosphonate to have vanishingly small  $K_{ows}$  at ambient pH.

Dimethyl methylphosphonate has a  $\log K_{ow}$  of -0.61 according to Krikorian<sup>8</sup>.

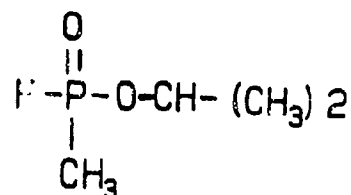


Dimethyl methylphosphonate

Diisopropyl methylphosphonate (DIMP) has  $\log K_{ow}$  values reported as 1.03 by Krikorian and Chorn<sup>8</sup> and 1.35 by Brueggemann<sup>9</sup>. The relationship between the  $\log K_{ow}$  values reported by Krikorian and Chorn for a series of phosphonates and the number of carbon atoms in these molecules, appears to be linear<sup>6</sup>. Regression of the data indicates an anomaly in the fit of DIMP, such that Krikorian and Chorn's value for  $\log K_{ow}$  is probably too low. Inclusion of Brueggemann's result in this relationship yields a much better fit and is therefore considered the more accurate value.



Diisopropyl methylphosphonate



GB

GB (isopropyl methylphosphonofluoridate) is a quick-acting nerve agent. It could not be tested in our laboratory, and  $K_{ow}$  values were not available in the literature. Rosenthal et al. reported chloroform/water, benzene/water, carbon tetrachloride/water and hexane/water partition coefficients of 31.2, 2.08, 0.84 and 0.20 respectively<sup>10</sup>. Such values can sometimes be used to estimate  $K_{ow}$  through solvent regression equations<sup>1</sup>. However, the results of such calculations were so divergent in the present instance that a credible value for  $K_{ow}$  could not be determined. It is known, however, that GB is volatile and hydrolyzes in water<sup>11</sup> and should therefore not pose a long-term environmental hazard.

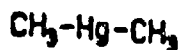
#### METHYLMERCURIES AND DIMETHYLMERCURY

Determination of the  $K_{ow}$  for metallic mercury and for methylmercury compounds presents several interesting problems. Mercury may be found in oxidation states 0, +1 and +2. Mercury metal (oxidation state 0) has limited solubility in water<sup>12</sup> and high volatility<sup>13</sup>. Shoichi and Sokichi<sup>14</sup> report  $K_{ow}$  values for metallic mercury of from 3.80 to 4.80, with values decreasing as a function of temperature in the range of 278 to 308 K. Mercury +1 and +2 salts may be methylated abiotically or microbially. In the methylated molecules the covalent bond between carbon and mercury resists hydrolytic cleavage<sup>15</sup>.  $K_{ow}$  values for mixed methylmercuric hydroxide and methylmercuric chloride are a result of equilibrium between the two species. The  $K_{ow}$  of the mixture in an aqueous medium appears to depend on salinity (chloride concentration) and pH<sup>16</sup>.

Dimethylmercury is a product of a microbial disproportionation reaction in which two methylmercury cations condense to yield un-ionized dimethylmercury and ionized mercury +2<sup>15</sup>.



Dimethylmercury is nearly insoluble in water and it has a high vapor pressure. These properties combine to give the compound a short residence time in aqueous systems and tend to make accurate determination of  $K_{ow}$  by conventional methods difficult. Wasik<sup>17</sup> was able to overcome these problems with an elegant method that determined the octanol/water partition coefficient and the Henry's law constant simultaneously. This system yielded the log  $K_{ow}$  value for dimethylmercury of 2.26 at 20° C.



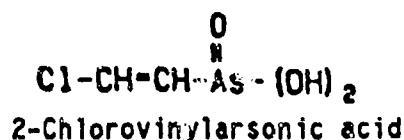
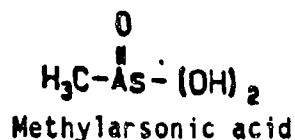
Dimethylmercury



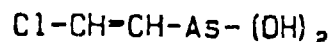
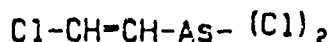
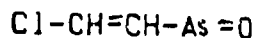
## COMPOUNDS OF ARSENIC

The compounds of arsenic for which  $K_{ow}$  values were requested are 2-chlorovinylarsonic acid, 2-chlorovinylarsonous acid, dimethylarsenic acid, lewisite, lewisite oxide and methylarsonic acid.

Methylarsonic acid should have an extremely low  $K_{ow}$  at pH 7 because it has a  $pK_a$  of only 4.1<sup>18</sup>. The similar compound, 2-chlorovinylarsonic acid, should hence have a low  $K_{ow}$ , as its chlorovinyl group is electron withdrawing,<sup>2</sup> making it an even stronger acid than methylarsonic acid.



The  $K_{ow}$  of lewisite cannot be determined since this compound is not stable in water. ARMY FM 3-9<sup>11</sup> reports that "The rate of hydrolysis is rapid for both vapor and dissolved lewisite and when the humidity is high lewisite hydrolyzes so rapidly that it is difficult to maintain a concentration sufficient to blister even unprotected skin." Lewisite oxide is the species formed when lewisite is hydrolyzed and then dried. It, in turn, is converted quantitatively to 2-chlorovinylarsonous acid when dissolved in water<sup>19</sup>. The latter compound represents the lewisite species actually found in water; it has a  $\log K_{ow}$  of -0.07 as determined in this Laboratory<sup>9</sup>.

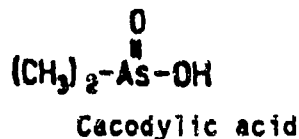
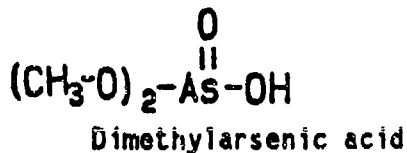


Lewisite oxide

Lewisite

2-Chlorovinylarsonous acid

Dimethylarsenic acid correctly denotes the diester of arsenic acid. However esters of this compound are highly unstable in water and diesters have never been reported<sup>18</sup>. This terminology has however, been used incorrectly to denote dimethylarsinic acid (cacodylic acid). Our experiments<sup>6</sup> have determined the latter compound to have a  $\log K_{ow}$  of -1.18.

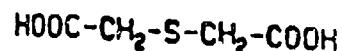
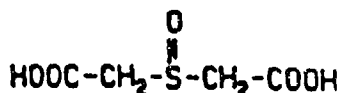
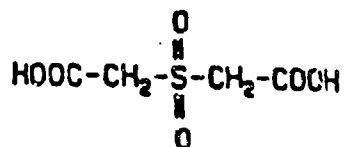


## ELEMENTAL METALS

With the exception of mercury, all the native metals listed are medium to high melting solids. Melting point has a substantial effect on aqueous solubility, and, as expected, the solubility of these elements is low.  $K_{ow}$  values are not available for any metal except mercury and their determination is not within the current capability of this laboratory.

# OTHER COMPOUNDS FOR WHICH K<sub>OW</sub> IS NOT APPLICABLE

Biscarboxymethyl sulfone, biscarboxymethyl sulfoxide and thiodiglycolic acid are putative or known environmental breakdown products of sulfur mustard; they differ only in the oxidation state of their sulfur atoms and are all in the form of anionic salts at pH>5. They are not susceptible to facile K<sub>OW</sub> measurement.

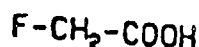
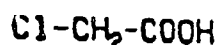


Biscarboxymethyl sulfone

Biscarboxymethyl sulfoxide

Thiodiglycolic acid

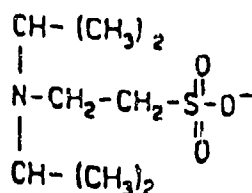
Bromide and chloride, being anions, are not susceptible to K<sub>OW</sub> determination. Chloroacetic acid and fluoroacetic acid have pK<sub>a</sub> values of 2.87 and 2.57<sup>20</sup>, so that they occur as anions at ambient pH.



Chloroacetic acid

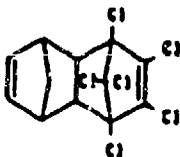
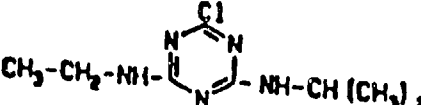
Fluoroacetic acid

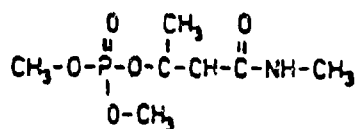
2-Diisopropylaminoethylsulfonate denotes the salt form of a sulfonic acid. Sulfonic acids as a class do not have determinable K<sub>OW</sub> values because they are very strong acids. They are reported to be the most water-soluble organic compounds known<sup>21</sup>.



2-Diisopropylaminoethylsulfonate.

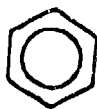
LOG K<sub>OW</sub> FOR COMPOUNDS FOR WHICH K<sub>OW</sub> VALUES ARE APPLICABLE (value listed first is considered most accurate)

COMPOUND	Log K <sub>OW</sub>	REFERENCE
	6.50	22 De Bruijn et al. 1989
	5.66	23 Geyer et al. 1984
	5.66	24 Kenaga 1980a
	5.3	25 USEPA 1986m
Aldrin		
	2.32	26 Rao and Davidson 1983
	2.64	23 Geyer et al. 1984
Atrazine		



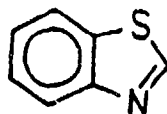
1.03 <sup>6</sup> Major 1988

Azodrin



2.01 <sup>28</sup> Valvani et al. 1980  
2.12 <sup>25</sup> USEPA 1986m  
2.13 <sup>27</sup> Sangster 1989

Benzene



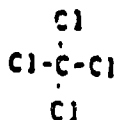
2.01 <sup>2</sup> Hansch and Leo 1979

Benzothiazole



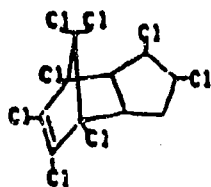
3.11 <sup>6</sup> Major 1988

Bicycloheptadiene



2.73 <sup>29</sup> Davies and Dobbs 1984  
2.73 <sup>23</sup> Geyer et al. 1984  
2.83 <sup>28</sup> Valvani et al. 1980  
2.64 <sup>30</sup> Neeley et al. 1974  
2.83 <sup>27</sup> Sangster 1989

Carbon tetrachloride



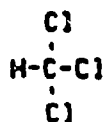
2.78 <sup>33</sup> Kadeg et al. 1986

Chlordane



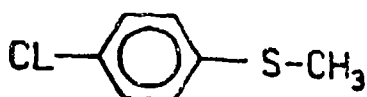
2.84 <sup>27</sup> Sangster 1989  
2.84 <sup>28</sup> Valvani et al. 1980  
2.98 <sup>31</sup> Tewari et al. 1982

Chlorobenzene

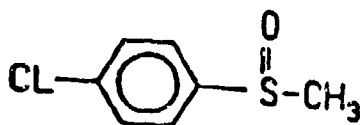


1.90 <sup>29</sup> Davies and Dobbs 1984  
1.96 <sup>28</sup> Valvani et al. 1980  
1.97 <sup>32</sup> Moriguchi 1975  
1.97 <sup>27</sup> Sangster 1989

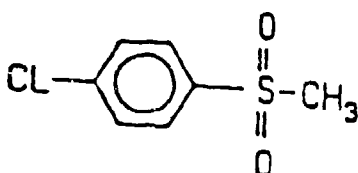
Chloroform



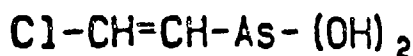
3.22 <sup>9</sup> Brueggemann 1979  
p-Chlorophenyl methyl sulfide



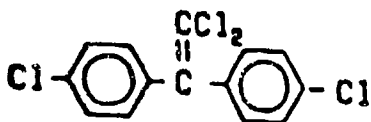
1.33 <sup>9</sup> Brueggemann 1979  
p-Chlorophenyl methyl sulfoxide



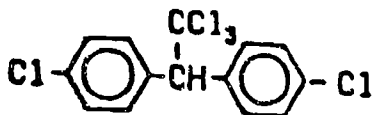
1.20 <sup>9</sup> Brueggemann 1979  
p-Chlorophenyl methyl sulfone



-0.07 <sup>6</sup> Major 1988  
2,Chlorovinylarsonous Acid



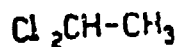
6.96 <sup>22</sup> De Bruijn et al. 1989  
5.69 <sup>26</sup> Rao and Davidson 1983  
5.60 (Mean value) <sup>33</sup> Kadek et al. 1986  
Dichlorodiphenyldichloroethylene (DDE)



6.91 <sup>22</sup> De Bruijn et al. 1989  
6.19 <sup>26</sup> Rao and Davidson 1983  
5.89 <sup>1</sup> Lyman et al. 1982  
Dichlorodiphenyltrichloroethane (DDT)

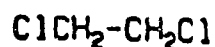


2.29 <sup>25</sup> USEPA 1986  
2.43 <sup>34</sup> USEPA 1985  
1,2-Dibromo-3-chloropropane



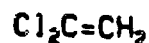
1.8 <sup>25</sup> USEPA 1986

1,1-Dichloroethane\_\_\_\_\_



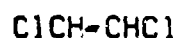
1.79 <sup>35</sup> Veith et al. 1983  
1.45 <sup>29</sup> Davies and Dobbs 1984  
1.48 <sup>2</sup> Hansch and Leo 1979

1,2-Dichloroethane\_\_\_\_\_



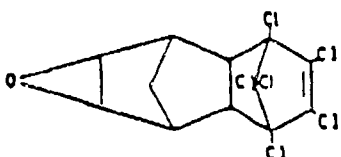
1.84 <sup>36</sup> Mabey et al. 1981

1,1-Dichloroethylene\_\_\_\_\_



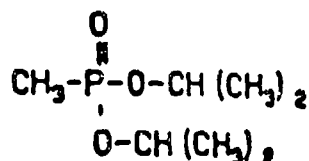
1.98 <sup>37</sup> Gossett et al. 1983

trans-1,2-Dichloroethylene\_\_\_\_\_



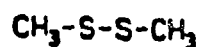
5.40 <sup>22</sup> De Bruijn et al. 1989  
4.32 <sup>29</sup> Davies and Dobbs 1984  
6.20 <sup>38</sup> Briggs 1981  
3.69 <sup>26</sup> Rao and Davidson 1983  
5.48 <sup>24</sup> Kenaga 1980  
3.50 <sup>25</sup> USEPA 1986

Dieldrin\_\_\_\_\_



1.35 <sup>9</sup> Brueggemann 1979

Diisopropyl methylphosphonate\_\_\_\_\_



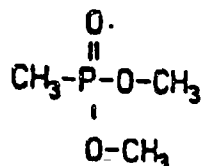
1.77 <sup>2</sup> Hansch and Leo 1979

Dimethyl disulfide\_\_\_\_\_



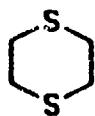
2.26 <sup>17</sup> Wasik 1978

Dimethylmercury\_\_\_\_\_

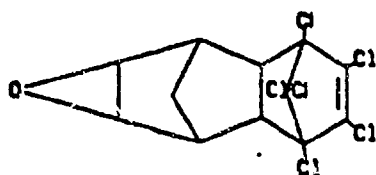


-0.61 <sup>8</sup> Krikorian 1987

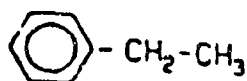
Dimethyl methylphosphonate\_\_\_\_\_



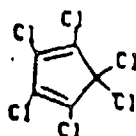
Dithiane (1,4 isomer) 1.85<sup>6</sup> Major 1988



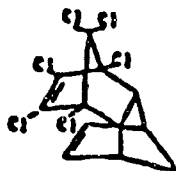
Endrin 5.20<sup>22</sup> De Bruijn et al. 1969  
6.34<sup>24</sup> Kenaga 1980



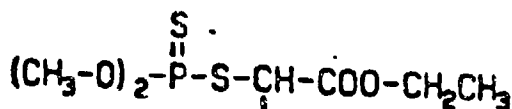
Ethylbenzene 3.15<sup>27</sup> Sangster 1989  
3.13<sup>31</sup> Tewari et al. 1982  
3.15<sup>32</sup> Moriguchi 1975



Hexachlorocyclopentadiene 5.04<sup>23</sup> Geyer et al. 1984



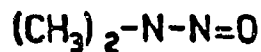
Isodrin 6.51<sup>1</sup> Lyman et al. 1982



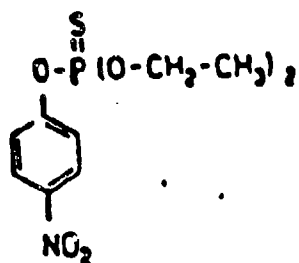
Malathion 2.89<sup>25</sup> USEPA 1986  
2.89<sup>2</sup> Hansch and Leo 1979  
2.89<sup>26</sup> Rao and Davidson 1983

Hg

Mercury 3.8 to 4.2 Shoichi<sup>13</sup> 1985

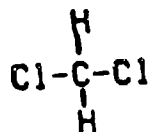


N-Nitrosodimethylamine -0.57<sup>2</sup> Hansch and Leo 1979



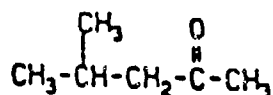
Parathion

3.9 <sup>38</sup> Briggs 1981  
3.8 <sup>26</sup> Rao and Davidson 1983



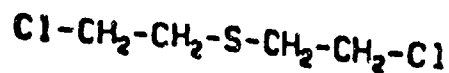
Methylene chloride

1.25 <sup>39</sup> Callahan et al. 1979  
1.30 <sup>25</sup> USEPA 1986  
1.31 <sup>27</sup> Sangster 1989



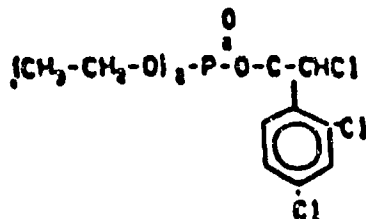
Methyl isobutyl ketone

1.53 <sup>6</sup> Major 1988



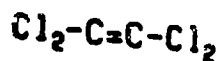
Sulfur mustard

1.37 <sup>25</sup> USEPA 1986m



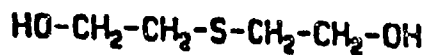
Supona

3.11 <sup>38</sup> Briggs 1981



Tetrachloroethylene

2.60 <sup>2</sup> Hansch and Leo 1979



Thiodiglyol

-0.08 <sup>6</sup> Major 1988



Thioxane (1,4 Oxathiane) 0.77<sup>6</sup> Major 1988

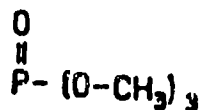


Toluene 2.73<sup>27</sup> Sangster 1989  
2.73<sup>25</sup> USEPA 1986  
2.58<sup>28</sup> Valvani et al. 1980  
2.65<sup>31</sup> Tewari et al. 1982  
2.69<sup>23</sup> Geyer et al. 1984  
2.69<sup>32</sup> Moriguchi 1975

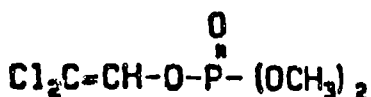
$\text{Cl}_3\text{C}-\text{CH}_3$  2.50<sup>25</sup> USEPA 1986  
2.47<sup>29</sup> Davies and Dobbs 1984  
 1,1,1-Trichloroethane \_\_\_\_\_

$\text{Cl}_2\text{CH}-\text{CH}_2\text{Cl}$  2.47<sup>25</sup> USEPA 1986  
 1,1,2-Trichloroethane \_\_\_\_\_

$\text{Cl}_2\text{C}=\text{CHCl}$  2.38<sup>25</sup> USEPA 1986  
2.29<sup>2</sup> Hansch and Leo 1979  
2.42<sup>35</sup> Veith et al. 1983  
3.3<sup>28</sup> Valvani et al. 1980  
3.3<sup>29</sup> Davies and Dobbs 1984  
3.3<sup>23</sup> Geyer et al. 1984  
2.29<sup>40</sup> Rogers et al 1980  
2.53<sup>29</sup> Tewari et al. 1982  
 Trichloroethylene \_\_\_\_\_



Trimethyl phosphate 0.52<sup>2</sup> Hansch and Leo 1979



Vapona 1.40<sup>2</sup> Hansch and Leo 1979



## REFERENCES:

1. Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt. 1982. Handbook of chemical property estimation methods: environmental behavior of organic compounds. McGraw-Hill Book Co., New York, NY.
2. Hansch, C. and A.J. Leo. 1979. Substituent constants for correlation analysis in chemistry and biology. John Wiley and Sons, New York, NY.
3. Harnisch, M., H.J. Mockel, and G. Schulze. 1983. Relationship between log  $K_{ow}$  shake-flask values and capacity factors derived from reversed-phase high performance liquid chromatography for n-alkylbenzenes and some reference substances. J. Chromatogr. 282:315-332.
4. Kosolapoff, G.M. 1950. Organophosphorus Compounds. John Wiley and Sons, Inc. New York, NY.
5. Fletcher, J.H., C.O. Dermer and R.B. Fox. 1974. Nomenclature of Organic Compounds Principles and Practice. American Chemical Society, Washington, DC.
6. Major, M. 1988. USABRDL Research Notebook Number 988.
7. Rosenblatt, D.H. and G.T. Davis. 1973. Laboratory Course in Organic Chemistry. Allyn and Bacon Inc. Boston, MA.
8. Krikorian, E.S. and T.A. Chorn. 1987. Determination of octanol/water partition coefficients of certain organophosphorus compounds using high performance liquid chromatography. Quant. Struct. Act. Relat. 6:65-69.
9. Brueggemann, E. 1979. USABRDL Laboratory Research Notebook Number 748.
10. Rosenthal, R.W., R. Proper and J. Epstein. 1965. The distribution of some phosphonofluoridates between organic solvents and water. J. Phys. Chem. 60: 1596-1598.
11. Military Chemistry and Chemical Compounds, U.S. Army FM 3-9, 1975.
12. Glew, D.N. and D.A. Hames. 1971. Aqueous nonelectrolyte solutions. Part X. Mercury solubility in water. Can. J. Chem. 49:3114-3118.
13. Shoichi, O. and S. Sokichi. 1984. Volatility of mercury in water. J. Hazard. Mater. 8:341-348.
14. Shoichi, O. and S. Sokichi. 1985. The 1-octanol/water partition coefficient of mercury. Bull. Chem. Soc. Jpn. 58:3401-3402.
15. Bodek, I.F., W.J. Lyman, W.F. Reehl and D.H. Rosenblatt. 1988. Environmental inorganic chemistry: Properties processes, and estimation methods. Pergamon Press. Elms Ford, NY.

16. Major, K.A., K.A. Bostian, and D.H. Rosenblatt. The octanol/water partition coefficient of methylmercuric chloride and methylmercuric hydroxide in pure water and salt solutions. In Draft.
17. Wasik, S.P. 1978. Partition of Organoelements in Octanol/Water/Air Systems. A.C.S. Symp. Ser. Organometallics and Organometalloids. Vol. 82:314-326.
18. Levander, O.A. and the National Academy of Sciences Subcommittee on Arsenic. 1977. Arsenic. National Academy of Sciences, Washington, DC.
19. Bossle P.C. 1988. Determination of lewisite contamination in environmental waters by high performance liquid chromatography. Paper presented to the Rocky Mountain Conference. July 1988.
20. Albert, A. and E.P. Serjeant. 1958. Ionization constants of acids and bases. John Wiley and Sons. New York, NY.
21. Morrison, T.M. and R.N. Boyd, 1970. Organic chemistry. Allyn and Bacon, Inc. Boston MA.
22. De Bruijn, J., F. Busser, W. Seinen and J. Hermens. 1989. Determination of octanol/water partition coefficients for hydrophobic organic chemicals with the "slow-stirring" method. Environ. Toxicol. Chem. 8(6):499-512.
23. Geyer, H., G. Politzki, and Freitag, D. 1984. Prediction of ecotoxicological behavior of chemicals: relationship between N-octanol/water partition coefficient and bioaccumulation of organic chemicals by *Alga Chlorella*. Chemosphere 13(2):269-284.
24. Kenaga, E.E. 1980. Correlation of bioconcentration factors of chemicals in aquatic and terrestrial organisms with their physical and chemical properties. Environ. Sci. Technol. 14(5):553-556.
25. U.S. Environmental Protection Agency (USEPA). 1986. Superfund public health evaluation manual. Prepared for USEPA by ICF Incorporated Washington, DC.
26. Rao, P.S.C. and Davidson, J. M. 1983. Estimation of pesticide retention and transformation parameters required in nonpoint source pollution models. Overcash, M.R. and J.M. Davidson, editors. Environmental impact of nonpoint source pollution. Ann Arbor Science Publishers, Inc., Ann Arbor, MI.
27. Sangster, J. 1989. Octanol-water partition coefficients of simple organic compounds. J. Phys. Ref. Data 18(3):1111-1229.
28. Valvani, S.C., S.H. Yalkowsky, and T. J. Roseman. 1980. Solubility and partitioning. IV. Aqueous solubility and octanol/water partition coefficients of liquid nonelectrolytes. J. Pharm. Sci. 70(5):502-505.
29. Davies, R.P. and A.J. Dobbs. 1984. The prediction of bioconcentration in fish. Water Res. 18(10):1253-1262.

30. Neely, W.B. 1974. Partition coefficient to measure bioconcentration potential of organic chemicals in fish. *Environ. Sci. Technol.* 8:1113.
31. Tewari, Y.B., M.M. Miller, S.P. Wasik, and D.E. Martire. 1982. Aqueous solubility and octanol/water partition coefficient of organic compounds at 25 degrees centigrade. *J. Chem. Eng. Data* 27:451-454.
32. Moriguchi, I. 1975. Quantitative structure-activity studies. I. Parameters relation to hydrophobicity. *Chem. Pharm. Bull.* 23(2):247-257.
33. Kadeg, R.D., Pavlou, S.P., and Duxbury, A.S. 1986. Elaboration of sediment normalization theory for non polar hydrophobic organic chemicals. U.S. Environmental Protection Agency, Criteria and Standards Division, Washington, DC.
34. U.S. Environmental Protection Agency (USEPA). 1985. Draft Health Advisory for 1,2-dibromo-3-chloropropane (DBCD). Office of Drinking Water. U.S. Environmental Protection Agency. Washington, DC.
35. Veith, G.D., D.J. Call, and L.T. Brooke. 1983. Structure-toxicity relationships for the fathead minnow, *Pimephales Promelas*: narcotic industrial chemicals. *Can. J. Fish Aquat. Sci.* 40:743-748.
36. Mabey, W.B., J.H. Smith, and R.T. Podoll. 1981. Aquatic fate process data for organic priority pollutants. USEPA, Monitoring and Data Support Division, Washington, D.C. EPA. Report No. EPA-440/4-81-014.
37. Gossett, R.W., D.A. Brown and D. Young. 1983. Prediction the bioaccumulation of organic compounds in marine organisms using octanol/water partition coefficients. *Mar. Pollut. Bull.* 14(10):387-392.
38. Briggs, G.G. 1981. Theoretical and experimental relationships between soil adsorption, octanol-water partition coefficients, water solubilities, bioconcentration factors, and the parachor. *J. Agric. Food Chem.* 29:1050-1059.
39. Callahan, M.A., M.W. Slimak, N.W. Gabel, I.P. May, C.F. Fowler, J.R. Freed, P. Jennings, R.L. Durfec, F.C. Whitmore, Maestri, W. R. Mabey, B.R. Holt, and C. Gould. 1979. Water-related environmental fate of 129 priority pollutants. Vol. I. EPA-440/4-79-029a. Office of Water Planning and Standards, Office of Water Waste Management, U.S. Environmental Protection Agency, Washington, DC.
40. Rogers, R.D., J.C. McFarlane and A.J. Cross. 1980. Adsorption and desorption of benzene in two soils and montmorillonite clay. *Environ. Sci. Technol.* 14(4):457-460.

APPENDIX A: LIST OF SUBSTANCES FOR WHICH  $K_{ow}$  VALUES WERE REQUESTED BY THE U.S. ARMY TOXIC AND HAZARDOUS MATERIALS AGENCY.

Aldrin	Dimethyl mercury (sicl)
Arsenic	Dithiane
Atrazine	Endrin
Azodrin	Ethyl benzene (sicl)
Benzene	Ethyl methyl phosphonate (sicl)
Benzothiazole	Ethyl methyl phosphonic acid (sicl)
Bicycloheptadiene	Fluoride
Biscarboxymethyl sulfone	Fluoroacetic acid
Biscarboxymethyl sulfoxide	GB; Sarin
Bromide	Hexachlorocyclopentadiene
Cadmium	Isodrin
Carbon tetrachloride	Isopropyl methyl phosphonic acid (sicl)
Chlordane	Isopropyl methyl phosphonate (sicl)
Chloride	Lead
Chloroacetic acid	Lewisite
Chlorobenzene	Lewisite oxide
Chloroform	Malathion
2-chlorovinyl arsonic acid (sicl)	Mercury
2-chlorovinyl arsonous acid (sicl)	Methylene chloride
p-Chlorophenyl methyl sulfide	Methyl arsonic acid (sicl)
p-Chlorophenyl methyl sulfoxide	Methyl isobutyl ketone
p-Chlorophenyl methyl sulfone	Methyl mercury salts (sicl)
Chromium	Methylphosphonic acid
Copper	Mustard
DDE	N-Nitrosodimethylamine
DDT	Parathion
1,2-Dibromo-3-chloropropane	Sulfur mustard
1,1-Dichloroethane	Supona
1,2-Dichloroethane	Tetrachloroethylene
1,1-Dichloroethylene	Thiodiglycol
1,2-Dichloroethylene	2,2-Thiodiglycolic acid
Dicyclopentadiene	Thioxane
Dieldrin	Toluene
2-(Diisopropylamino)-n-ethyl sulfonate (sicl)	1,1,1-Trichloroethane
2-(Diisopropylamino)-n-ethanethiol (sicl)	1,1,2-Trichloroethane
Diisopropylmethylphosphonate (sicl)	Trichloroethylene
Dimethyl disulfide	Trimethyl phosphate
Dimethyl methyl phosphonate (sicl)	Vapona
Dimethyl arsenic acid (sicl)	

# DISTRIBUTION LIST

## No. of Copies

4	Commander U.S. Army Medical Research and Development Command ATTN: SGRD-RMI-S Fort Detrick, Frederick, MD 21701-5012
2	Commander, U.S. Army Biomedical Research and Development Laboratory, ATTN: SGRD-UBZ-IL Fort Detrick, Frederick, MD 21701-5010
2	Defense Technical Information Center (DTIC) ATTN: DTIC-DDAC Cameron Station Alexandria, VA 22304-6145
1	Commandant Academy of Health Sciences, U.S. Army ATTN: HSHA-DCD Fort Sam Houston, TX 78234-5000
1	Chief U.S. Army Environmental Hygiene Agency Regional Division, West Fitzsimmons Army Medical Center Aurora, CO 80045-5000
1	Chief U.S. Army Environmental Hygiene Agency Regional Division, North Fort George G. Meade, MD 20755-5000
1	Chief U.S. Army Environmental Hygiene Agency Regional Division, South Building 180 Fort McPherson, GA 30330-5000
1	Commander U.S. Army Health Services Command ATTN: HSPA-P Fort Sam Houston, TX 78234-5000
1	Commandant U.S. Army Academy of Health Sciences ATTN: Chief, Environmental Quality Branch Preventive Medicine Division (HSHA-IPM) Fort Sam Houston, TX 78234-5000

1 U.S. Army Engineers  
Division, Huntsville  
106 Wynn Drive  
Huntsville, AL 35807-4301

1 Chief  
Army Environmental Office  
ATTN: ENVR-EP  
The Pentagon  
Room 1E669  
Washington, DC 20310-2600

1 Commander  
U.S. Naval Facilities Engineering Command  
Environmental Quality Division  
200 Stovall Street  
Alexandria, VA 22332-2300

1 Headquarters  
Air Force Engineering Service Center  
ATTN: RDV  
Tyndall Air Force Base, FL 32403-6001

1 Commander  
U.S. Army Materiel Command  
ATTN: AMSCG  
5001 Eisenhower Avenue  
Alexandria, VA 22333-2300

1 Commander  
U.S. Army Environmental Hygiene Agency  
ATTN: HSDH-AD-L  
Aberdeen Proving Ground, MD 21010-5000

1 Dean  
School of Medicine  
Uniformed Services University of the Health Sciences  
4301 Jones Bridge Road  
Bethesda, MD 20014-5000

1 Commander  
U.S. Army Materiel Command  
ATTN: AMCEN-A  
5001 Eisenhower Avenue  
Alexandria, VA 22333-2300

1 HQDA(DASG-PSP-E)  
5111 Leesburg Pike  
Falls Church, VA 22041-3258

1 HQDA(DAEN-RDM)  
20 Massachusetts Avenue, NW  
Washington, DC 20314-5000

1 Commander  
U.S. Army Toxic and Hazardous Materials Agency  
ATTN: CETH-TE-D (Mr. Bartell)  
Aberdeen Proving Ground, MD 21010-5401